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SOLUTIONS WITH SINGULAR INITIAL DATA FOR A MODEL OF ELECTROPHORETIC SEPARATION

BY

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ABSTRACT. Unique global strong solutions of a Cauchy problem arising in electrophoretic separation are constructed with arbitrary initial data in L^1, thus generalizing an earlier global existence result. For small diffusion coefficients, the solutions can be viewed as approximate solutions for the corresponding zero-diffusion Riemann problem.

1. Introduction. Electrophoresis describes various processes by which proteins and other biological materials are separated in solution by an imposed electric field ([5], [6], [12]). The modeling equations for electrophoretic separation developed in [12] are of advection-diffusion type and relate the electric field $E = E(x,t)$ to the chemical species concentrations $u_i = u_i(x,t)$, $i = 1, \ldots, m$, as follows:

$$(u_i)_t = d_i(u_i)_{xx} + [z_i\Omega_i E u_i]_x, \tag{1.1a}$$

$$E_x = (-e/\epsilon)\sum_{k=1}^{m} z_k u_k \tag{1.1b}$$

Here t is nonnegative and x lies in a suitable domain of $\mathbf{R}$ which depends on the particular separation technique used. Meanwhile e, ϵ and each d_i, Ω_i, and z_i are constants: e is the molar charge and ϵ is the permittivity of the solvent, while d_i and Ω_i are the diffusivity and mobility of the ith species. Each z_i is $+1$ or -1 depending on whether the ith species is a positive or negative ion. For further background on the physical significance of equations (1.1), please see [6] or [12].

Here, as in [4] and [6], we focus on a particular separation technique known as isotachophoresis, or ITP, in which the reaction column is long and connected at both ends to large electrolyte reservoirs which negate the influence of reactions occurring at the electrodes. This makes the concentrations constant at the column ends and effectively renders the system infinitely long ([6], [12]). Thus x varies over the entire real line in (1.1) and the concentrations satisfy the fixed Dirichlet boundary conditions

$$u_i(-\infty) = \alpha_i, \quad u_i(+\infty) = \beta_i. \tag{1.1c}$$

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As in [4] and [6] we assume the following conditions which also are appropriate for ITP:

(1.2) $$(u_i)_x(\pm\infty, t) = 0,$$

(1.3) $$\sum_{i=1}^{m} z_i\alpha_i = \sum_{i=1}^{m} z_i\beta_i = 0.$$

Condition (1.3), in particular, is a natural condition to impose in light of the separation mechanism and it plays an important role in [4] and the present work. Condition (1.2) is appropriate due to the asymptotically constant behavior of the concentrations; its connection with various types of initial data will be discussed in the next section.

The remaining boundary conditions apply to the electric field E. It is often the case that the electric current I is constant through the medium; as in [4] and [6] we assume that here. We will see that as in [4] it is appropriate to assume that $U(x,t) \equiv (-e/\epsilon)\sum_{k=1}^{m} z_k u_k$ is in $L^1(\mathbf{R})$. Integrating (1.1b) we then have that

$$E(x,t) = \int_{-\infty}^{x} U(y,t)dy + C(t).$$

In fact it is shown in [4] that C does not depend on time: the development in section 2 of [4] shows that the constant current condition allows us to set

(1.4) $$E(x,t) = (-e/\epsilon)\int_{-\infty}^{x}\sum_{k=1}^{m} z_k u_k(y,t)dy + E_-$$

where E_- is a constant that can be determined explicitly by (1.1c), the value of I, and the choice of initial conditions

(1.5) $$u_i(x,0) = u_i^0.$$

Similarly it can be shown that $E(+\infty, t)$ is in fact equal to a specifiable constant E_+ (independent of time). We refer the reader to [4, section 2] for more details of the derivation of (1.4). Here we only need to know that these details allow us to use (1.4) to define E. Thus we can eliminate (1.1b), plug (1.4) into (1.1a), and thus rewrite (1.1) as a system of m integro-differential equations in the unknown u_i.

In [4] equations (1.1) were handled by first defining functions $w_i(x)$ as follows:

(1.6) $$w_i(x) = \begin{cases} \alpha_i, & x \leqq -1 \\ \ell_i(x), & -1 < x < 1 \\ \beta_i, & x \geqq 1, \end{cases}$$

where ℓ_i is such that $\alpha_i \leqq \ell_i \leqq \beta_i$ and ℓ_i makes w_i a C^∞ function of x. Note that $(w_i)_x \in C_0^\infty \equiv C_0^\infty(\mathbf{R})$ and that by (1.3) $\sum_{k=1}^{m} z_k w_k \in C_0^\infty$ as well. Setting $u_i = v_i + w_i$ and plugging into (1.1) we obtain the following equations in v_i:

(1.7) $$(v_i)_t = d_i(v_i)_{xx} + c_i[E(v+w)(v_i+w_i)]_x + d_i(w_i)_{xx}$$

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where $c_i = z_i\Omega_i$ and $E(v+w)$ is defined by (1.4) with u_k replaced by $v_k + w_k$. Global strong solutions of (1.7) were found in [4] with initial data $v_i^0 \equiv v_i(0) \in W^{2,1}(\mathbf{R})$. In the next sections we will extend this result to allow for singular initial data, establishing global strong solutions for arbitrary $v_i^0 \in L^1(\mathbf{R})$. With the u_i thus defined in terms of v_i and w_i, we note that it is indeed appropriate to assume that $\sum_{k=1}^m z_k u_k$ is in $L^1(\mathbf{R})$, so that E in (1.7) can be defined by (1.4) as discussed above.

The assumption $v_i^0 \in L^1(\mathbf{R})$ includes as a special case $v_i^0 = f(x) + g(x)$ where $f(x) \in W^{n,1} \equiv W^{n,1}(\mathbf{R})$ with $n \geqq 2$ and $g(x) \in L_0^1(\mathbf{R})$, where $L_0^1(\mathbf{R})$ is the set of all functions in L^1 with compact support. Included in the set of all such $f(x)+g(x)$ are locally piecewise constant functions, a class of initial data that arises in practice when (1.1) is considered with each $d_i = 0$ ([8]). Thus one application of our theory is the production (for small d_i) of approximate solutions to the hyperbolic problem for a wide class of initial data.

Note that for $v_i^0 = f(x) + g(x)$ as specified above, the boundary conditions (1.1c) and (1.2) are automatically satisfied by $u_i(x,0) = v_i^0 + w_i$. We will show in the next section that for each $t > 0$ $u_i(x,t) \in W^{n,1}$ for all $n \geqq 2$, thus u_i will satisfy the conditions (1.1c), (1.2) for all $t \geqq 0$.

One can regard (1.7) as a pure Cauchy problem, however, independent of (1.1) and the associated boundary conditions. There have been a number of results in recent years on nonlinear parabolic problems with initial data in L^p, see e.g. [3], [9], [10], [13], [14] (in addition to these applications, the Benjamin-Bona-Mahony equation was discussed with L^p initial data in [2]). We remark that the boundary conditions (1.1c) and (1.2) are satisfied for arbitrary initial data v_i^0 in L^1 when t is positive.

2. **Local Existence.** If, for a vector valued function $f = (f_1, \dots, f_m)$ with $f_i \in L^1$ we define

$$F(f) = (-e/\epsilon)\int_{-\infty}^{x} \sum_{k=1}^{m} z_k f_k(y)dy, \tag{2.1}$$

then we note that

$$E(v+w) = F(v) + E(w) \tag{2.2}$$

where $E(w)$ is obtained by replacing u_k by w_k in the right-hand side of (1.4). Let $W_i(t)$ denote the semigroup generated by $d_i(\cdot)_{xx}$, then equations (1.7) have the corresponding integral equations

$$\begin{aligned} v_i(t) = {} & W_i(t)v_i^0 + G_i(w,t) \\ & + c_i \int_0^t W_i(t-s)[E\big(v(s)+w\big)v_i(s) + F\big(v(s)\big)w_i]_x\, ds \end{aligned} \tag{2.3}$$

where F, E are as in (2.1), (2.2) and

$$G_i(w,t) = \int_0^t W_i(t-s)[c_i E(w)w_i + d_i(w_i)_x]_x\, ds. \tag{2.4}$$

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Our goal in this section is to solve (2.3) by a contraction-mapping method for $0 \leqq t \leqq T$ with $T > 0$ suitably chosen.

By the Sobolev embedding theorems ([1], [7]) for each integer $n \geqq 0$ there is a constant C_n such that for all $f \in W^{n+1,1}$

$$\|f\|_{n,\infty} \leqq C_n \|f\|_{n+1,1} \tag{2.5}$$

where $\|\cdot\|_{n,\infty}$ denotes the norm on $C_B^n(\mathbf{R})$. Direct differentiation of the explicit kernel for $W_i(t)$ shows that there is a constant K_i such that for all $f \in W^{n,1}$ and all $t \in (0, 1]$

$$\|W_i(t)f\|_{n+1,1} \leqq K_i t^{-\frac{1}{2}} \|f\|_{n,1}. \tag{2.6}$$

As in [13] or [14], by considering (2.6) first on dense subsets of smooth functions, we have for all $f \in W^{n,1}$ that

$$\lim_{t \downarrow 0} t^{\frac{1}{2}} \|W_i(t)f\|_{n+1,1} = 0. \tag{2.7}$$

We note, in fact, that many of the techniques that follow are based on arguments that appeared in [13] and [14], also later in [3].

Since $(w_i)_x$ and $\sum_{k=1}^m z_k w_k$ are both in C_0^∞ it follows that $[c_i E(w) w_i]_x$ is in C_0^∞, hence $G_i(w, t)$ is in $W^{j,1}$ for all $j \geqq 0$. In fact, there exists a constant M, depending only on e, ϵ, c_i, d_i, and the supremum norms of w_i, $(w_i)_x$, $(w_i)_{xx}$, such that $|G_i(w, t)| \leqq MT$ for all $t \in [0, T]$. For fixed $v_i^0 \in W^{n,1}$ it follows by this last remark and (2.6) and (2.7) that there exist positive numbers α, β, T such that $\beta \downarrow 0$ as $T \downarrow 0$ and

$$\|W_i(t)v_i^0 + G_i(w, t)\|_{n,1} \leqq \alpha, \tag{2.8a}$$

$$t^{\frac{1}{2}} \|W_i(t)v_i^0 + G_i(w, t)\|_{n+1,1} \leqq \beta, \tag{2.8b}$$

for all $t \in (0, T]$; here $\alpha = \|v_i^0\|_{n,1} + MT$.

For α, β, T as above let M be the space of all curves $v(t) = \big(v_1(t), \ldots, v_m(t)\big)$ such that for each i

(1) $v_i : [0, T] \longrightarrow W^{n,1}$ is continuous and $\|v_i(t)\|_{n,1} \leqq 2\alpha$, $0 \leqq t \leqq T$;
(2) $v_i : (0, T] \longrightarrow W^{n+1,1}$ is continuous and $t^{\frac{1}{2}} \|v_i(t)\|_{n+1,1} \leqq 2\beta$, $0 < t \leqq T$.

M is a nonempty complete metric space with metric ρ where, for $v, u \in M$

$$\rho(u, v) = \sup_{1 \leqq i \leqq m} \sup_{0 < t \leqq T} \left\{ \|v_i(t) - u_i(t)\|_{n,1}, t^{\frac{1}{2}} \|v_i(t) - u_i(t)\|_{n+1,1} \right\}.$$

Let $(Sv)(t) = \big((S_1 v_1)(t), \ldots, (S_m v_m)(t)\big)$ where for each i $(S_i v_i)(t)$ is the right-hand side of (2.3). In the proof of the following result we obtain a fixed point of S, hence a local solution of (2.3), by showing that S is a contraction on M.

THEOREM 2.1. *For each integer* $n \geqq 0$ *and each* $v_i^0 \in W^{n,1}$ *there exists a* $T > 0$ *such that* (2.3) *has a unique solution* $v_i \in C([0,T];\, W^{n,1}) \cap C\big((0,T];\, W^{n+1}\big)$.

PROOF. Let $\gamma = |-e/\epsilon|$, then from (1.4) and (2.1) note that for $v \in M$

$$\|E\big(v(t)+w\big)\|_\infty \leqq \gamma \left[\sum_{k=1}^{m} \|v_k(t)\|_1 + \left\|\sum_{k=1}^{m} z_k w_k\right\|_1\right] + E_- \leqq \gamma(2\alpha m) + L_1 \tag{2.9}$$

where L_1 depends only on γ, E_-, and the w_i; meanwhile

$$\|F\big(v(t)\big)\|_\infty \leqq \gamma \sum_{k=1}^{m} \|v_k(t)\|_1 \leqq \gamma(2\alpha m), \tag{2.10}$$

and, if $F_x\big(v(t)\big) = [F\big(v(t)\big)]_x$, and $D_j f$ denotes $(d^j f)/(dx^j)$, $0 \leqq j \leqq n$

$$\|D_j F_x\big(v(t)\big)\|_1 \leqq \gamma \sum_{k=1}^{m} \|v_k(t)\|_{j,1} \leqq \gamma(2\alpha m), \tag{2.11}$$

similarly

$$\|D_j E_x\big(v(t)+w\big)\|_1 \leqq \gamma(2\alpha m) + L_2 \tag{2.12}$$

where L_2 depends only on γ, E_-, and the w_i.

If $1 \leqq j \leqq n$ we see from (2.5) that

$$\begin{aligned} \|D_j F\big(v(t)\big)\|_\infty = \|D_{j-1} F_x\big(v(t)\big)\|_\infty &\leqq \gamma \sum_{k=1}^{m} \|D_{j-1} v_k(t)\|_\infty \\ &\leqq \gamma \sum_{k=1}^{m} C_n \|v_k(t)\|_{n,1} \leqq \gamma C_n(2\alpha m) \end{aligned} \tag{2.13}$$

and similarly

$$\|D_j E\big(v(t)+w\big)\|_\infty \leqq \gamma C_n(2\alpha m) + L_3 \tag{2.14}$$

where L_3 depends only on γ, E_-, and the w_i. Meanwhile it is clear that for each i and for $0 \leqq j \leqq n$

$$\|D_j v_i(t)\|_\infty \leqq C_{n+1} \|v_i(t)\|_{n+1,1} \leqq C_{n+1}(2\beta t^{-\frac{1}{2}}) \tag{2.15}$$

and that

$$\|D_j (v_i)_x(t)\|_1 \leqq \|v_i(t)\|_{n+1,1} \leqq 2\beta t^{-\frac{1}{2}}. \tag{2.16}$$

Using (2.9)–(2.16) we thus have for all $v \in M$ and all $i = 1, \ldots, m$ that

$$
\begin{aligned}
(2.17)\qquad & \|[E(v(t)+w)v_i(t) + F(v(t))w_i]_x\|_{n,1} \\
&\leqq \|E_x(v(t)+w)v_i(t)\|_{n,1} + \|E(v(t)+w)(v_i)_x(t)\|_{n,1} \\
&\quad + \|F_x(v(t))w_i\|_{n,1} + \|F(v(t))(w_i)_x\|_{n,1} \\
&\leqq \sum_{k=0}^{n}\sum_{j=0}^{k}\begin{bmatrix} k \\ j \end{bmatrix} \|D_j E_x(v(t)+w)\|_1 \|D_{k-j} v_i(t)\|_\infty \\
&\quad + \|E(v(t)+w)\|_\infty \|(v_i)_x(t)\|_1 \\
&\quad + \sum_{k=1}^{n}\sum_{j=1}^{k}\begin{bmatrix} k \\ j \end{bmatrix} \|D_j E(v(t)+w)\|_\infty \|D_{k-j}(v_i)_x(t)\|_1 \\
&\quad + \sum_{k=0}^{n}\sum_{j=0}^{k}\begin{bmatrix} k \\ j \end{bmatrix} \|D_j F_x(v(t))\|_1 \|D_{k-j} w_i\|_\infty \\
&\quad + \|F(v(t))\|_\infty \|(w_i)_x\|_1 \\
&\quad + \sum_{k=1}^{n}\sum_{j=1}^{k} \|D_j F(v(t))\|_\infty \|D_{k-j}(w_i)_x\|_1 \\
&\leqq N_1(\gamma(2\alpha m) + L_2)C_{n+1}(2\beta t^{-\frac{1}{2}}) \\
&\quad + (\gamma(2\alpha m) + L_2)(2\beta t^{-\frac{1}{2}}) + N_2(\gamma C_n(2\alpha m) + L_3)(2\beta t^{-\frac{1}{2}}) \\
&\quad + N_3\gamma(2\alpha m) + N_4\gamma(2\alpha m) + N_5\gamma C_n(2\alpha m)
\end{aligned}
$$

where N_1 and N_2 depend only on n while N_3, N_4 and N_5 depend only on n and the w_i. Hence there exist constants A, B and C depending only on γ, E_-, n, m, and the w_i such that

$$(2.18)\qquad \|[E(v(t)+w)v_i(t) + F(v(t))w_i]_x\|_{n,1} \leqq (\alpha A + B)\beta t^{-\frac{1}{2}} + \alpha C.$$

Hence from (2.18) and (2.8) we see that for all $v \in M$ and $t \in [0, T]$

$$(2.19)\quad \|(Sv)(t)\|_{n,1} \leqq \alpha + |c_i| \int_0^t [(\alpha A + B)\beta s^{-\frac{1}{2}} + \alpha C]ds \leqq \alpha + |c_i|[(\alpha A + B)2\beta T^{\frac{1}{2}} + \alpha CT]$$

where we have used the fact that each D_j commutes with $W_i(t)$ for all $j \geqq 0$ and hence $W_i(t)$ is a contraction on $W^{n,1}$.

Now if c, $d \in (0, 1)$ a simple scaling argument (see [13]) shows that

$$(2.20)\qquad \int_0^t (t-s)^{-c}s^{-d}\,ds = t^{1-c-d}\int_0^1 (1-s)^{-c}s^{-d}\,ds.$$

Combining (2.20) with (2.8), (2.18), (2.19) and (2.6) we see that

$$
\begin{aligned}
(2.21)\quad \|(Sv)(t)\|_{n+1,1} &\leqq \beta + |c_i| \int_0^t K_i(t-s)^{-\frac{1}{2}}[(\alpha A + B)\beta s^{-\frac{1}{2}} + \alpha C]ds \\
&\leqq \beta + |c_i|K_i\left[\alpha C T^{\frac{1}{2}} + \beta(\alpha A + B)\int_0^1 (1-s)^{-\frac{1}{2}}s^{-\frac{1}{2}}\,ds\right].
\end{aligned}
$$

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Recalling that we can arrange that $\beta \downarrow 0$ as $T \downarrow 0$, it is now clear from (2.19) and (2.21) that we can select T and β small enough so that S maps M into M. A similar argument shows that S is a contraction on M, thus completing the proof of Theorem 2.1. We note in particular that the theorem includes the case $n = 0$, thus allowing the initial data v_i^0 to be arbitrary functions in L^1.

3. **Global Existence and Regularity.** If we set $n = 0$ in Theorem 2.1, so that $v_i \in L^1$, then note that, for $0 < t \leqq T$ with T as in the theorem, the local solution $u_i(t)$ is in $W^{1,1}$. Fixing $t_0 \in (0, T)$ and setting $v_i^0 = v_i(t_0)$, Theorem 2.1 can now be applied with $n = 1$ to obtain a solution $\bar{v}_i(t)$ of (2.3) on some interval $[0, T_0]$ such that $\overline{v_i} \in C\left((0, T_0];\, W^{2,1}\right)$. If we now replace T by $\min\{T, T_0\}$ we see by the uniqueness assertion of Theorem 2.1 that $v_i(t) = \overline{v_i}(t - t_0)$ for $t_0 < t \leqq T$. As t_0 is an arbitrary element of $(0, T)$ we can conclude that $v_i \in C\left((0, T];\, W^{2,1}\right)$. But in [4] global strong solutions of (1.7) were found for arbitrary initial data v_i^0 in $W^{2,1}$. Using arguments similar to those above and applying Theorem 2.1 of [4] we thus have established the following global existence result.

THEOREM 3.1. *For arbitrary $v_i^0 \in L^1$ equations* (1.7) *have unique global strong solutions $v_i \in C\left([0, +\infty);\, L^1\right) \cap C^1\left((0, +\infty);\, W^{2,1}\right)$.*

It is now clear that we can continue the bootstrap process described above for $n \geqq 1$, and regularity in t follows from regularity in x by standard arguments (see e.g. [11, p. 42]). We thus can improve Theorem 3.1 as follows:

THEOREM 3.2. *For arbitrary $v_i^0 \in L^1$ equations* (1.7) *have unique global strong solutions, $v_i \in C\left([0, +\infty);\, L^1\right) \cap C^j\left((0, +\infty);\, W^{n,1}\right)$ for all $j \geqq 1$ and all $n \geqq 1$.*

4. **Remarks.** We note that in [10], solutions with singular initial data were produced for conservation laws arising in gas dynamics. For small enough initial data in $L^2 \cap L^\infty$, the solutions could be extended globally. In the present work, we also construct solutions that can be viewed as approximate solutions to a Riemann problem for small values of the d_i. We are able to avoid both boundedness and size restrictions on v_i^0 because of the special structure of our equations.

In [8], solutions of (1.1) were found with each $d_i = 0$ with the additional assumptions of electroneutrality ($\epsilon = 0$) and monotonicity of the initial data. One could relax these assumptions by constructing solutions in the limit as $d_i \downarrow 0$ of the solutions guaranteed by Theorem 3.1. We hope to investigate this limit in a future paper.

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